ABSTRACT

The present invention provides methods for the generation of virtual libraries of compounds. These compounds are generated *in silico*. The present invention encompasses methods for tracking the addition of fragments, use of reagents, and transformations performed. Further, methods for interfacing the information necessary to generate libraries of compounds with instrumentation that conducts the actual synthesis of the compounds are provided. Also provided are methods for the *in silico* docking of the library compounds to identified target molecules of interest.

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